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2-(1,3-Benzothiazol-2-ylsulfanyl)-*N*-(2-methylphenyl)acetamide

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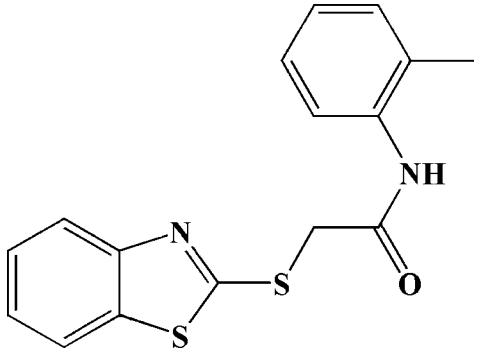
Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.100; data-to-parameter ratio = 17.5.

In the title molecule, $C_{16}H_{14}N_2OS_2$, the benzene ring and the benzo[*d*]thiazole mean plane form a dihedral angle of 75.5 (1)°. The acetamide group is twisted by 47.7 (1)° from the attached benzene ring. In the crystal, molecules related by translation along the *a* axis are linked into chains through N—H···O hydrogen bonds.

Related literature

For the crystal structures of similar compounds, see: Gao *et al.* (2007); Zhao *et al.* (2009). For the medical activity of heterocyclic derivatives containing the acetamide group, see: Fallah-Tafti *et al.* (2011); Shams *et al.* (2011)



Experimental

Crystal data

$C_{16}H_{14}N_2OS_2$
M_r = 314.41
Monoclinic, $P2_1/n$
a = 4.7957 (8) Å
b = 27.496 (4) Å
c = 10.9906 (13) Å
β = 97.048 (4)°
V = 1438.3 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 113 K
0.22 × 0.06 × 0.06 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min} = 0.923, T_{max} = 0.978
14718 measured reflections
3421 independent reflections
2923 reflections with $I > 2\sigma(I)$
R_{int} = 0.055

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.100
S = 1.06
3421 reflections
195 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.81 (2)	2.10 (2)	2.906 (2)	168 (2)

Symmetry code: (i) $x+1, y, z$.

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV5340).

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supplementary materials

Acta Cryst. (2012). E**68**, o3138 [doi:10.1107/S1600536812042109]

2-(1,3-Benzothiazol-2-ylsulfanyl)-*N*-(2-methylphenyl)acetamide

Yue Sun, Xiao-Jun Wang and Peng-Wu Zheng

Comment

Acylamide compounds have gained widely attention due to their the important medical activity. Recently, the synthesis and medical activities of some heterocyclic derivatives containing the acylamide moiety have been reported (Fallah-Tafti *et al.*, 2011; Shams *et al.*, 2011). Now the title compound, 2-(benzo[*d*]thiazol-2-ylthio)-N-*o*-tolylacetamide, was synthesized and its crystal structure was reported.

The molecular structure of title compound and the atom-mumbering scheme are shown in Fig. 1. The molecule contain a benzene ring and benzo[*d*]thiazole ring. The dihedral angle between the benzene ring and benzo[*d*]thiazole ring is 75.5°. The acetamide group is twisted at 47.7 (1)° from the attached benzene ring. C1 atom attached to the benzene ring is coplanar to the benzene ring with an r.m.s deviation of 0.0046 Å. As a result of π–π conjugation, the C_{sp^2}—S bond [S1—C10 = 1.745 (2) Å] is significantly shorter than the C_{sp^3}—S bond [S1—C9 = 1.812 (2) Å]. These values compare with the values of 1.772 (3) and 1.801 (2) Å reported in the literature (Gao *et al.*, 2007; Zhao *et al.*, 2009).

The crystal structure is stablized by the intermolecular N—H···O hydrogen bond (Table 1) interaction.

Experimental

The title compound was synthesized by the reaction of the benzo[*d*]thiazol-2-thiol with 2-methylphenyl carbamic chloride in the refluxing ethanol. Crystals of (I) suitable for single-crystal X-ray analysis were grown by slow evaporation of a solution in chloroform–ethanol (1:1).

Refinement

Atom H1 attached to N atom was located on a difference map and refined isotropically. Other H atoms were positioned geometrically (C—H = 0.95–0.99 Å), and refined as riding, with U_{iso}(H) = 1.2–1.5U_{eq}(C).

Computing details

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear* (Rigaku/MSC, 2005); data reduction: *CrystalClear* (Rigaku/MSC, 2005); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

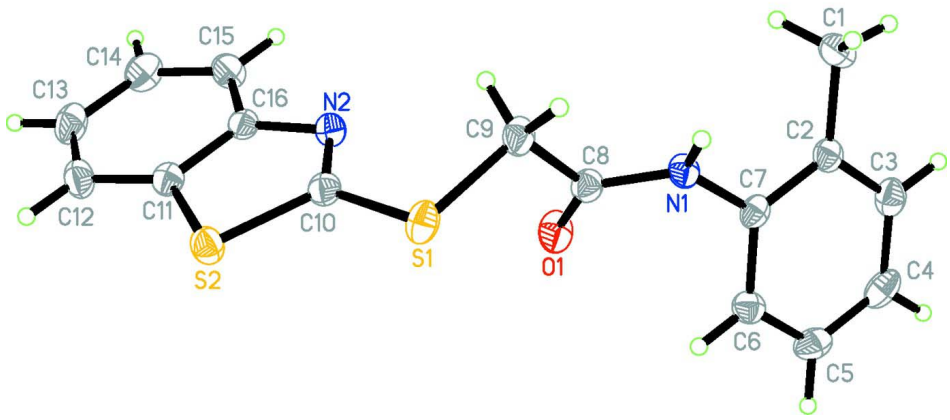

Figure 1

View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 60% probability level.

2-(1,3-Benzothiazol-2-ylsulfanyl)-*N*-(2-methylphenyl)acetamide

Crystal data

$C_{16}H_{14}N_2OS_2$
$M_r = 314.41$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
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$b = 27.496\ (4)$ Å
$c = 10.9906\ (13)$ Å
$\beta = 97.048\ (4)°$
$V = 1438.3\ (4)$ Å^3
$Z = 4$
$F(000) = 656$
$D_x = 1.452$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4445 reflections
$\theta = 1.5–27.9°$
$\mu = 0.37$ mm^{-1}
$T = 113$ K
Prism, colourless
0.22 × 0.06 × 0.06 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.22 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min} = 0.923$, $T_{max} = 0.978$
14718 measured reflections
3421 independent reflections
2923 reflections with $I > 2\sigma(I)$
$R_{int} = 0.055$
$\theta_{max} = 27.9°$, $\theta_{min} = 1.5°$
$h = -6\rightarrow6$
$k = -36\rightarrow36$
$l = -14\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.100$
$S = 1.06$
3421 reflections
195 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0351P)^2 + 0.5795P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$

$\Delta\rho_{max} = 0.33$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.48672 (11)	0.112141 (18)	0.29125 (5)	0.02069 (14)
S2	0.16105 (11)	0.158557 (18)	0.47479 (5)	0.01966 (14)
O1	0.1342 (3)	0.09883 (5)	0.03414 (14)	0.0233 (3)
N1	0.5406 (4)	0.08369 (6)	−0.04653 (15)	0.0162 (4)
N2	0.1583 (3)	0.19259 (6)	0.25292 (15)	0.0168 (3)
C1	0.6969 (4)	0.10401 (7)	−0.2868 (2)	0.0224 (5)
H1A	0.7119	0.1064	−0.3747	0.034*
H1B	0.8819	0.0965	−0.2424	0.034*
H1C	0.6295	0.1350	−0.2573	0.034*
C2	0.4933 (4)	0.06418 (7)	−0.26509 (18)	0.0170 (4)
C3	0.3715 (4)	0.03516 (7)	−0.36122 (19)	0.0212 (4)
H3	0.4183	0.0407	−0.4416	0.025*
C4	0.1835 (4)	−0.00162 (7)	−0.3421 (2)	0.0230 (5)
H4	0.1010	−0.0206	−0.4092	0.028*
C5	0.1159 (4)	−0.01059 (7)	−0.2249 (2)	0.0216 (4)
H5	−0.0119	−0.0359	−0.2115	0.026*
C6	0.2356 (4)	0.01747 (7)	−0.12783 (19)	0.0181 (4)
H6	0.1916	0.0112	−0.0473	0.022*
C7	0.4210 (4)	0.05501 (7)	−0.14794 (18)	0.0157 (4)
C8	0.3912 (4)	0.10278 (7)	0.03867 (18)	0.0174 (4)
C9	0.5622 (4)	0.13057 (7)	0.14044 (18)	0.0203 (4)
H9A	0.5228	0.1658	0.1296	0.024*
H9B	0.7645	0.1254	0.1346	0.024*
C10	0.2600 (4)	0.15837 (7)	0.32579 (18)	0.0171 (4)
C11	−0.0382 (4)	0.21033 (7)	0.43540 (18)	0.0172 (4)
C12	−0.2001 (4)	0.23768 (8)	0.50696 (19)	0.0221 (4)
H12	−0.2147	0.2290	0.5896	0.026*
C13	−0.3391 (4)	0.27784 (8)	0.4536 (2)	0.0243 (5)
H13	−0.4518	0.2970	0.5004	0.029*
C14	−0.3167 (4)	0.29069 (8)	0.3323 (2)	0.0243 (5)
H14	−0.4140	0.3185	0.2980	0.029*
C15	−0.1551 (4)	0.26352 (7)	0.26125 (19)	0.0217 (4)
H15	−0.1412	0.2724	0.1786	0.026*

C16	−0.0131 (4)	0.22287 (7)	0.31355 (18)	0.0157 (4)
H1	0.710 (5)	0.0869 (8)	−0.034 (2)	0.019 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0214 (3)	0.0197 (3)	0.0205 (3)	0.0055 (2)	0.0010 (2)	−0.0037 (2)
S2	0.0230 (3)	0.0202 (3)	0.0161 (3)	0.0031 (2)	0.0038 (2)	0.00153 (19)
O1	0.0109 (7)	0.0304 (8)	0.0289 (9)	−0.0010 (6)	0.0032 (6)	−0.0092 (7)
N1	0.0101 (8)	0.0202 (9)	0.0186 (9)	−0.0016 (7)	0.0025 (7)	−0.0035 (7)
N2	0.0168 (8)	0.0176 (8)	0.0163 (8)	0.0011 (6)	0.0029 (7)	−0.0007 (7)
C1	0.0207 (11)	0.0236 (11)	0.0238 (11)	−0.0007 (8)	0.0068 (9)	0.0036 (9)
C2	0.0151 (10)	0.0168 (9)	0.0193 (10)	0.0035 (7)	0.0032 (8)	0.0004 (8)
C3	0.0252 (11)	0.0211 (10)	0.0175 (10)	0.0063 (8)	0.0026 (9)	0.0001 (8)
C4	0.0268 (11)	0.0177 (10)	0.0223 (11)	0.0021 (8)	−0.0059 (9)	−0.0055 (8)
C5	0.0179 (10)	0.0170 (10)	0.0292 (12)	−0.0022 (8)	0.0003 (9)	−0.0004 (9)
C6	0.0156 (10)	0.0184 (10)	0.0205 (10)	0.0009 (8)	0.0032 (8)	0.0015 (8)
C7	0.0129 (9)	0.0148 (9)	0.0191 (10)	0.0031 (7)	0.0003 (8)	−0.0021 (8)
C8	0.0156 (10)	0.0167 (9)	0.0199 (10)	0.0000 (8)	0.0027 (8)	−0.0022 (8)
C9	0.0139 (10)	0.0233 (10)	0.0243 (11)	−0.0013 (8)	0.0051 (9)	−0.0074 (8)
C10	0.0151 (9)	0.0182 (9)	0.0178 (10)	−0.0023 (8)	0.0019 (8)	−0.0027 (8)
C11	0.0158 (10)	0.0177 (9)	0.0179 (10)	0.0000 (8)	0.0017 (8)	−0.0015 (8)
C12	0.0214 (11)	0.0269 (11)	0.0189 (10)	0.0001 (9)	0.0070 (9)	−0.0041 (9)
C13	0.0196 (11)	0.0253 (11)	0.0284 (12)	0.0023 (9)	0.0050 (9)	−0.0088 (9)
C14	0.0229 (11)	0.0201 (10)	0.0294 (12)	0.0062 (8)	0.0010 (9)	−0.0004 (9)
C15	0.0226 (11)	0.0217 (10)	0.0215 (11)	0.0025 (8)	0.0056 (9)	0.0026 (8)
C16	0.0137 (9)	0.0159 (9)	0.0179 (10)	−0.0013 (7)	0.0027 (8)	−0.0021 (7)

Geometric parameters (Å, º)

S1—C10	1.745 (2)	C4—H4	0.9500
S1—C9	1.812 (2)	C5—C6	1.383 (3)
S2—C11	1.739 (2)	C5—H5	0.9500
S2—C10	1.760 (2)	C6—C7	1.398 (3)
O1—C8	1.232 (2)	C6—H6	0.9500
N1—C8	1.353 (2)	C8—C9	1.511 (3)
N1—C7	1.427 (2)	C9—H9A	0.9900
N1—H1	0.81 (2)	C9—H9B	0.9900
N2—C10	1.292 (2)	C11—C12	1.392 (3)
N2—C16	1.395 (2)	C11—C16	1.402 (3)
C1—C2	1.505 (3)	C12—C13	1.382 (3)
C1—H1A	0.9800	C12—H12	0.9500
C1—H1B	0.9800	C13—C14	1.396 (3)
C1—H1C	0.9800	C13—H13	0.9500
C2—C3	1.394 (3)	C14—C15	1.385 (3)
C2—C7	1.397 (3)	C14—H14	0.9500
C3—C4	1.388 (3)	C15—C16	1.395 (3)
C3—H3	0.9500	C15—H15	0.9500
C4—C5	1.388 (3)		

C10—S1—C9	101.26 (9)	O1—C8—N1	123.37 (18)
C11—S2—C10	88.47 (9)	O1—C8—C9	121.60 (17)
C8—N1—C7	123.97 (16)	N1—C8—C9	115.02 (16)
C8—N1—H1	116.7 (16)	C8—C9—S1	112.61 (14)
C7—N1—H1	119.1 (16)	C8—C9—H9A	109.1
C10—N2—C16	109.77 (16)	S1—C9—H9A	109.1
C2—C1—H1A	109.5	C8—C9—H9B	109.1
C2—C1—H1B	109.5	S1—C9—H9B	109.1
H1A—C1—H1B	109.5	H9A—C9—H9B	107.8
C2—C1—H1C	109.5	N2—C10—S1	126.43 (15)
H1A—C1—H1C	109.5	N2—C10—S2	116.76 (14)
H1B—C1—H1C	109.5	S1—C10—S2	116.81 (11)
C3—C2—C7	117.84 (18)	C12—C11—C16	121.74 (18)
C3—C2—C1	121.07 (18)	C12—C11—S2	128.98 (16)
C7—C2—C1	121.10 (18)	C16—C11—S2	109.27 (14)
C4—C3—C2	121.46 (19)	C13—C12—C11	117.73 (19)
C4—C3—H3	119.3	C13—C12—H12	121.1
C2—C3—H3	119.3	C11—C12—H12	121.1
C3—C4—C5	119.99 (19)	C12—C13—C14	121.17 (19)
C3—C4—H4	120.0	C12—C13—H13	119.4
C5—C4—H4	120.0	C14—C13—H13	119.4
C6—C5—C4	119.65 (19)	C15—C14—C13	121.1 (2)
C6—C5—H5	120.2	C15—C14—H14	119.5
C4—C5—H5	120.2	C13—C14—H14	119.5
C5—C6—C7	120.11 (19)	C14—C15—C16	118.57 (19)
C5—C6—H6	119.9	C14—C15—H15	120.7
C7—C6—H6	119.9	C16—C15—H15	120.7
C2—C7—C6	120.93 (18)	N2—C16—C15	124.56 (18)
C2—C7—N1	119.92 (17)	N2—C16—C11	115.72 (17)
C6—C7—N1	119.15 (17)	C15—C16—C11	119.72 (17)

C7—C2—C3—C4	0.2 (3)	C9—S1—C10—N2	6.5 (2)
C1—C2—C3—C4	−179.95 (18)	C9—S1—C10—S2	−173.28 (11)
C2—C3—C4—C5	−0.9 (3)	C11—S2—C10—N2	−0.15 (16)
C3—C4—C5—C6	0.4 (3)	C11—S2—C10—S1	179.60 (12)
C4—C5—C6—C7	0.7 (3)	C10—S2—C11—C12	−179.2 (2)
C3—C2—C7—C6	0.9 (3)	C10—S2—C11—C16	0.11 (15)
C1—C2—C7—C6	−178.92 (17)	C16—C11—C12—C13	0.5 (3)
C3—C2—C7—N1	179.88 (17)	S2—C11—C12—C13	179.73 (16)
C1—C2—C7—N1	0.1 (3)	C11—C12—C13—C14	−0.3 (3)
C5—C6—C7—C2	−1.4 (3)	C12—C13—C14—C15	0.2 (3)
C5—C6—C7—N1	179.61 (17)	C13—C14—C15—C16	−0.2 (3)
C8—N1—C7—C2	134.3 (2)	C10—N2—C16—C15	179.80 (19)
C8—N1—C7—C6	−46.7 (3)	C10—N2—C16—C11	−0.1 (2)
C7—N1—C8—O1	−3.0 (3)	C14—C15—C16—N2	−179.45 (18)
C7—N1—C8—C9	178.09 (17)	C14—C15—C16—C11	0.4 (3)
O1—C8—C9—S1	50.5 (2)	C12—C11—C16—N2	179.32 (17)
N1—C8—C9—S1	−130.60 (16)	S2—C11—C16—N2	−0.1 (2)
C10—S1—C9—C8	−100.06 (15)	C12—C11—C16—C15	−0.5 (3)

C16—N2—C10—S1	−179.59 (14)	S2—C11—C16—C15	−179.92 (15)
C16—N2—C10—S2	0.1 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.81 (2)	2.10 (2)	2.906 (2)	168 (2)

Symmetry code: (i) *x*+1, *y*, *z*.